



FAIR combination of diverse experimental data in specialized repositories - Challenges and possible solutions

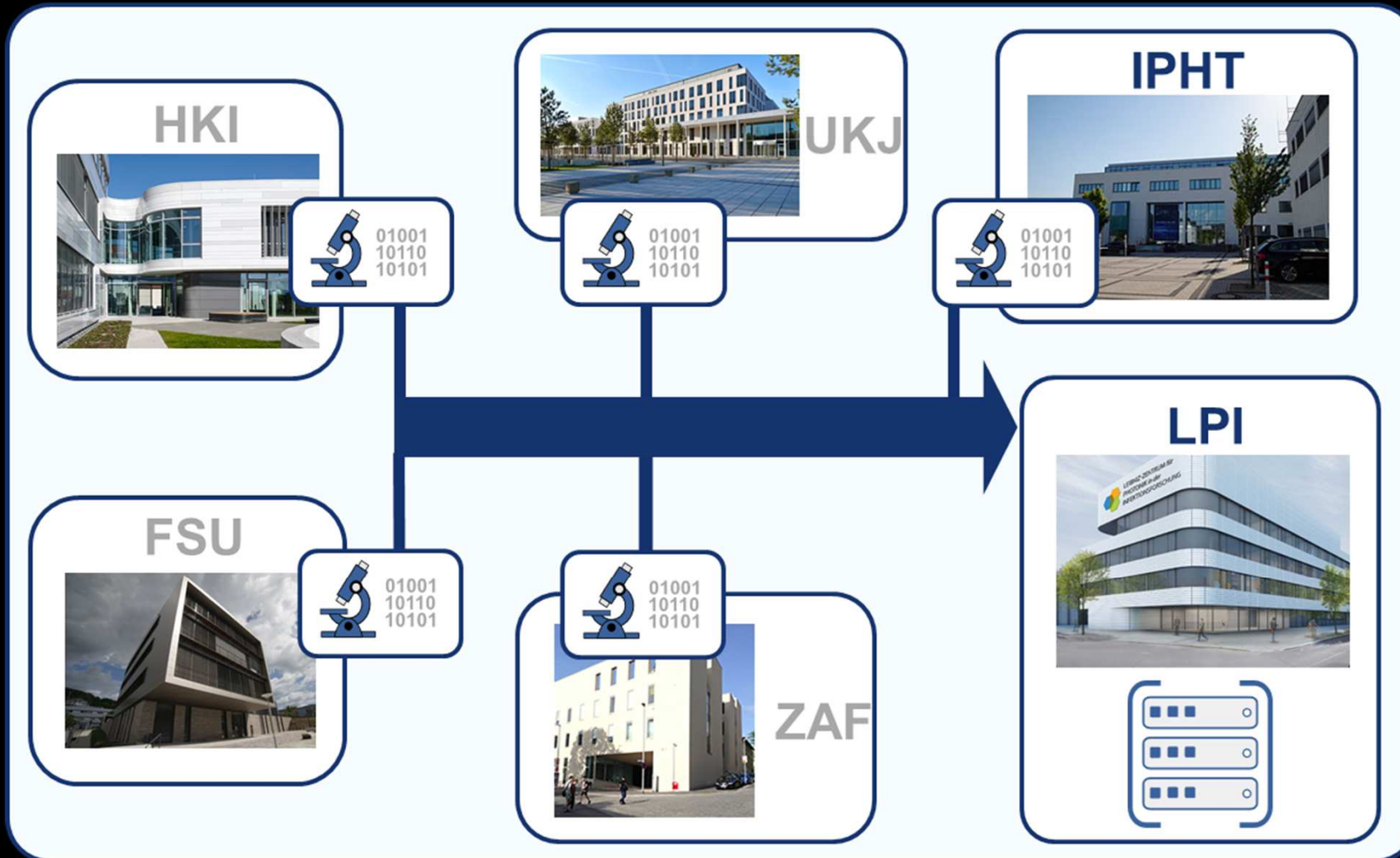
Laserlab-Europe / ELI Workshop

Better data for better science

29th of October 2021

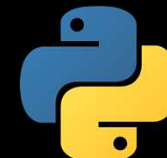
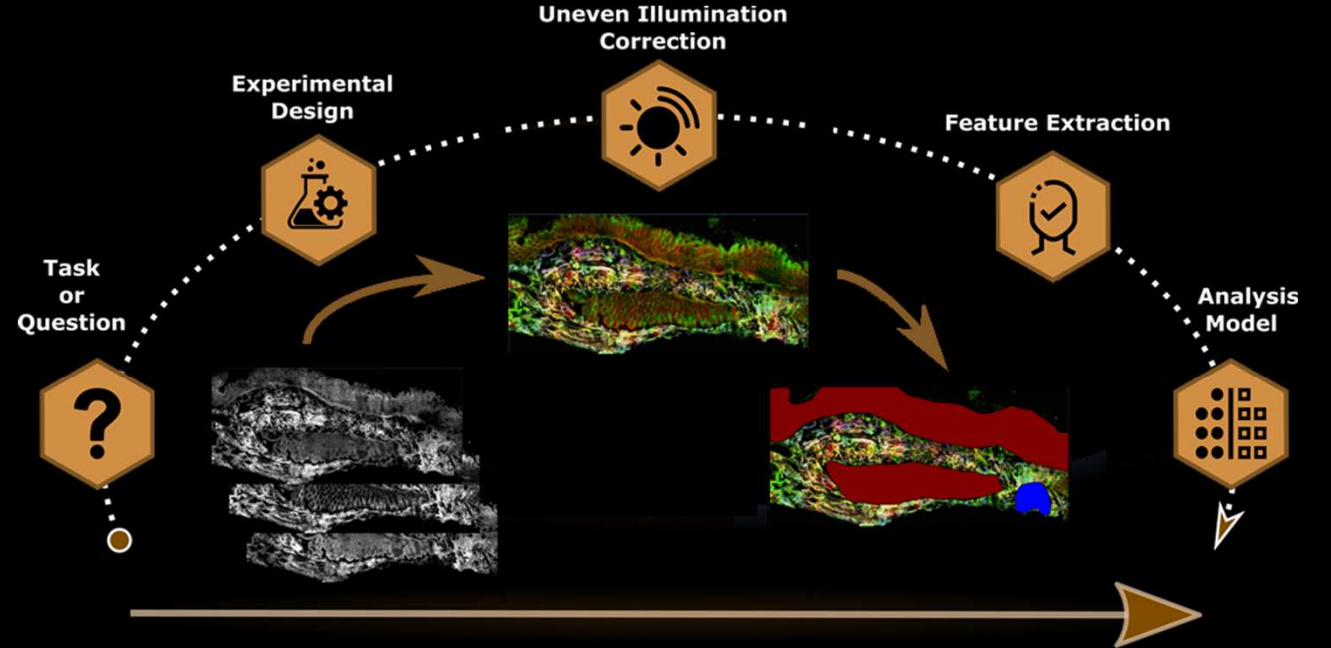
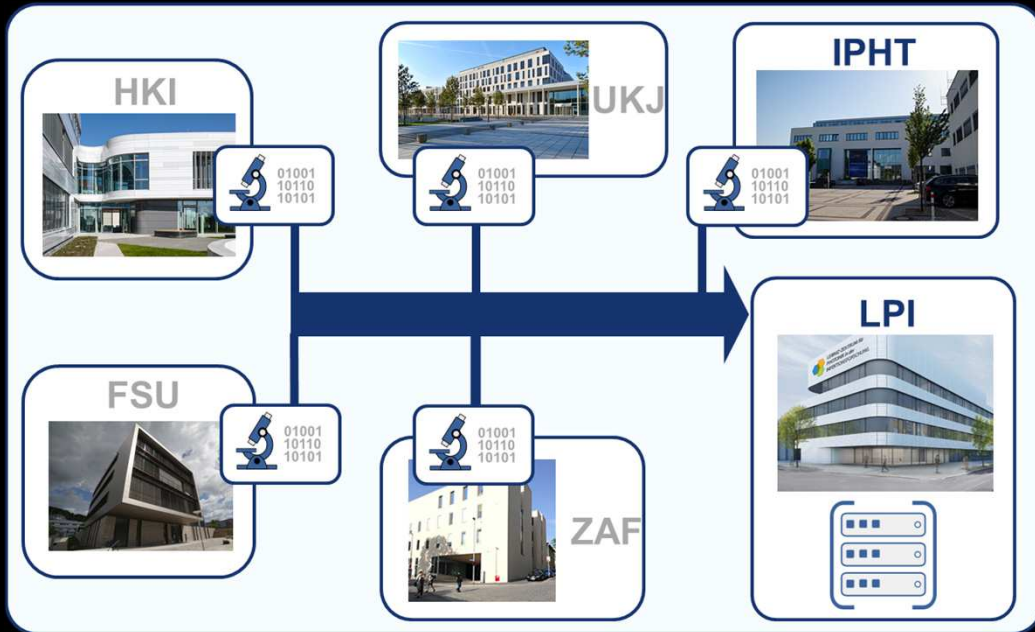
Julian Hniopek

Introduction & Motivation

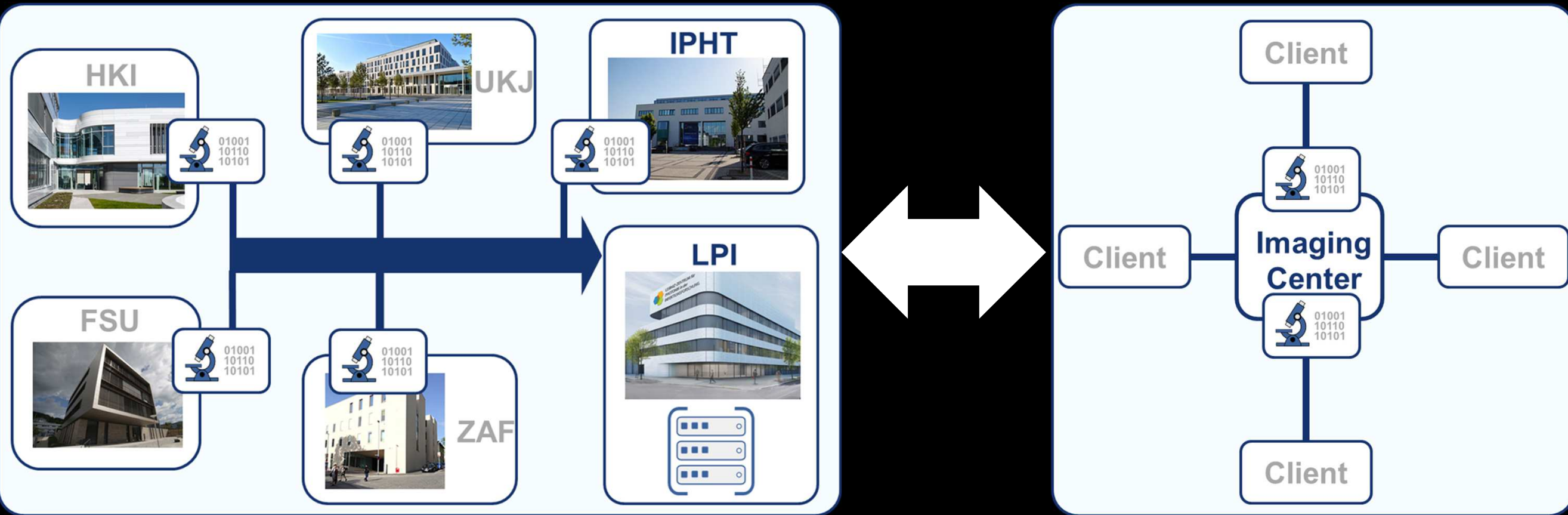


- Multidisciplinary consortium in Jena
- Distributed over different locations
- Very different requirements and typical usecases
- Central data management

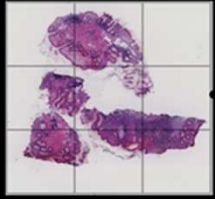
Introduction & Motivation



Introduction & Motivation



Current State

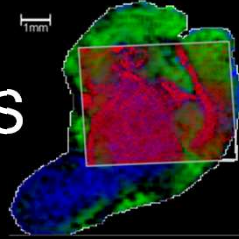


Staining techniques

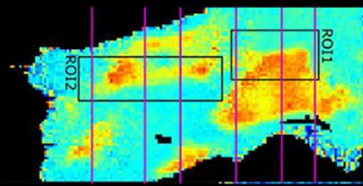
Patient characteristics



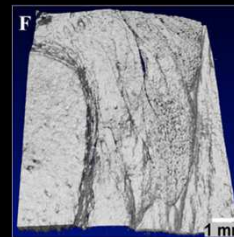
MALDI MS imaging



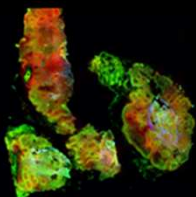
Fluorescence imaging / FLIM



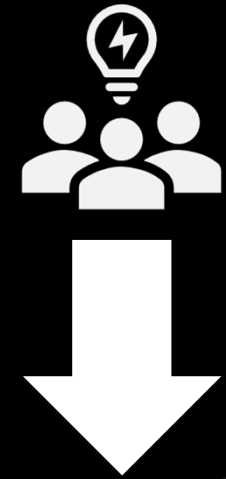
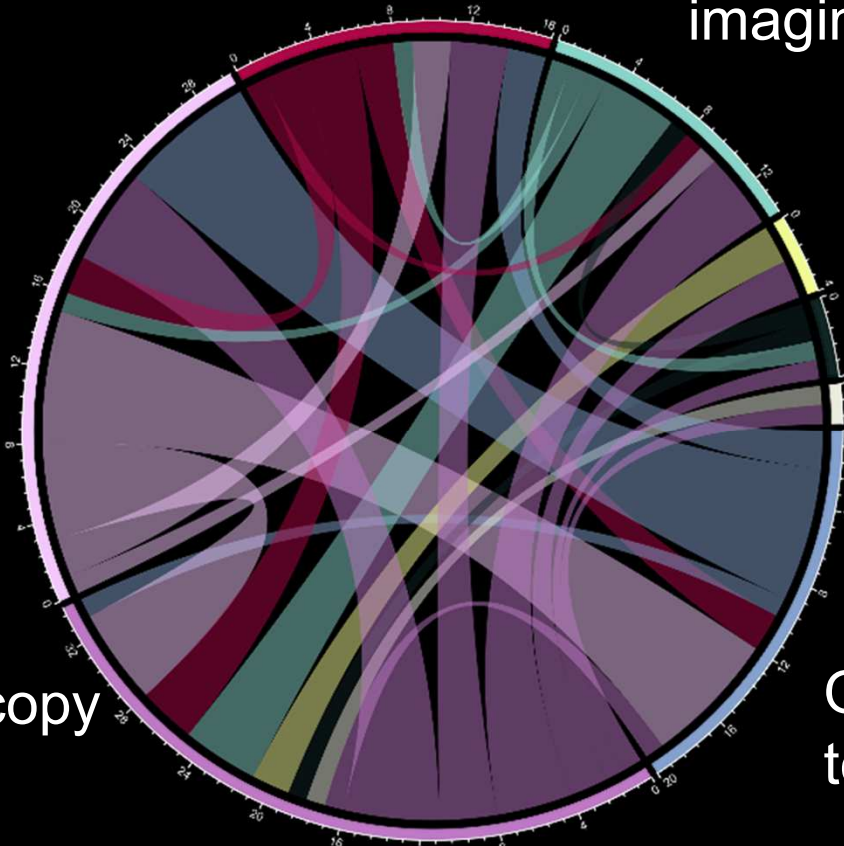
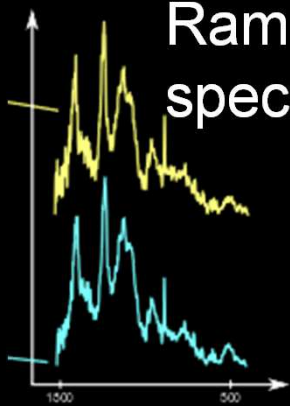
Optical coherence tomography



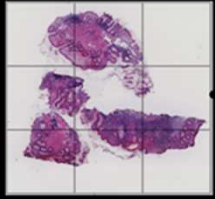
Multimodal imaging



Raman spectroscopy



Current State

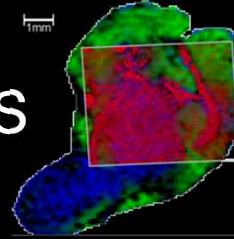


Staining techniques

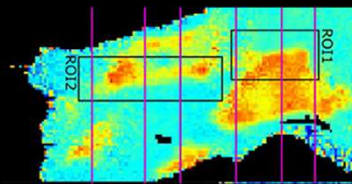
Patient characteristics



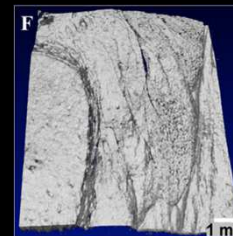
MALDI MS imaging



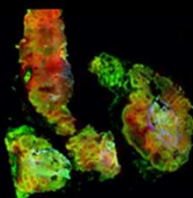
Fluorescence imaging / FLIM



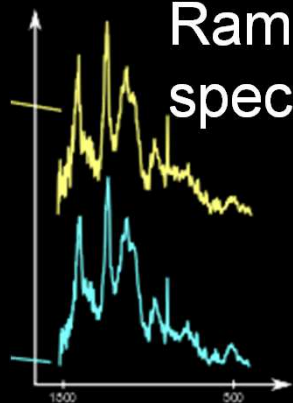
Optical coherence tomography



Multimodal imaging



Raman spectroscopy



Findable



Accessible

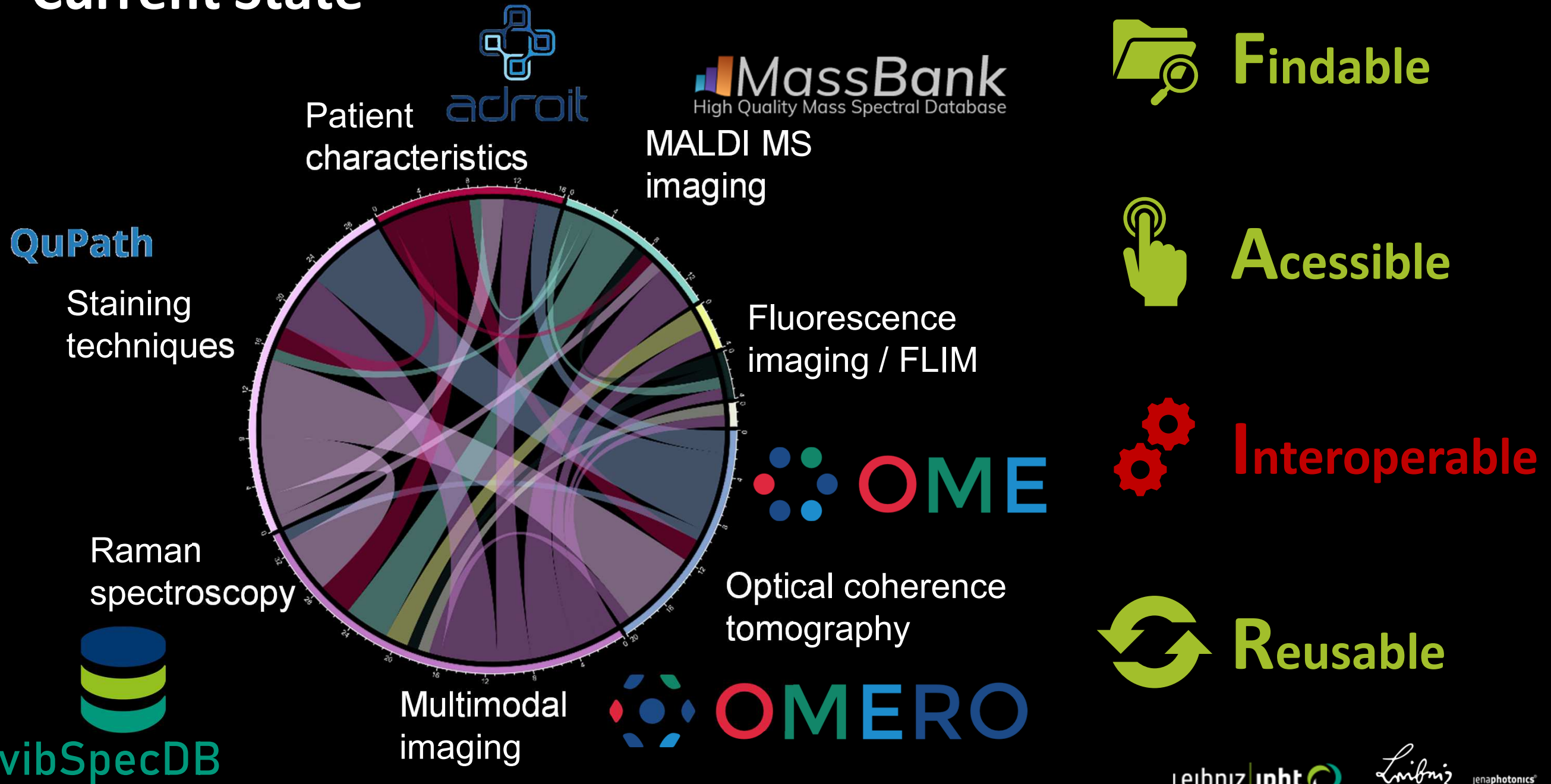


Interoperable

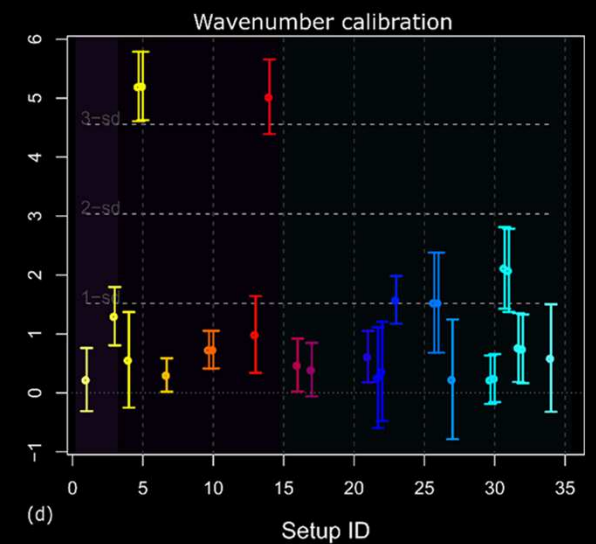
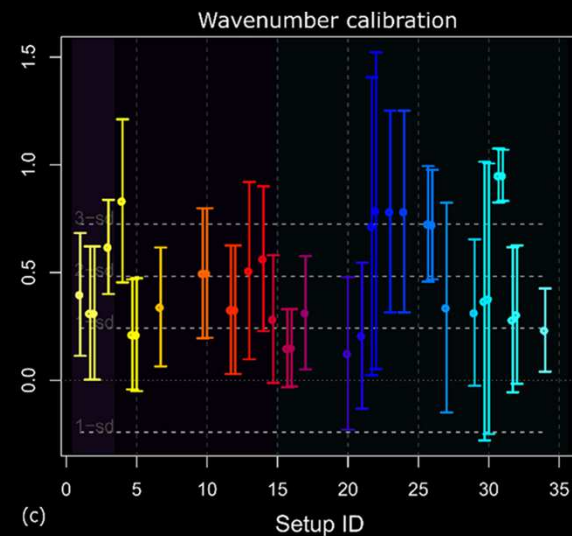
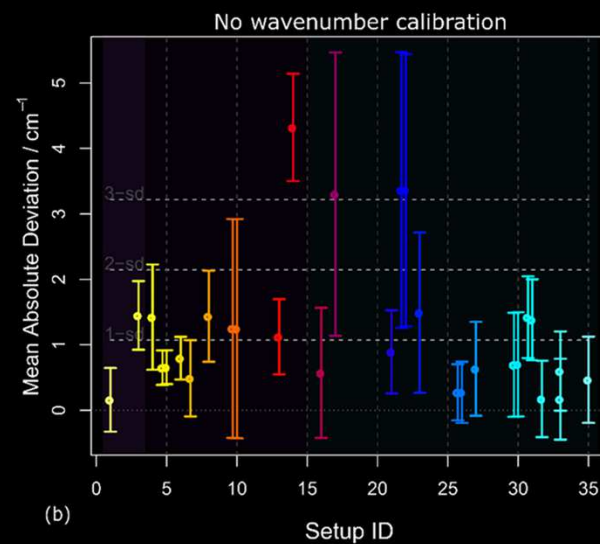
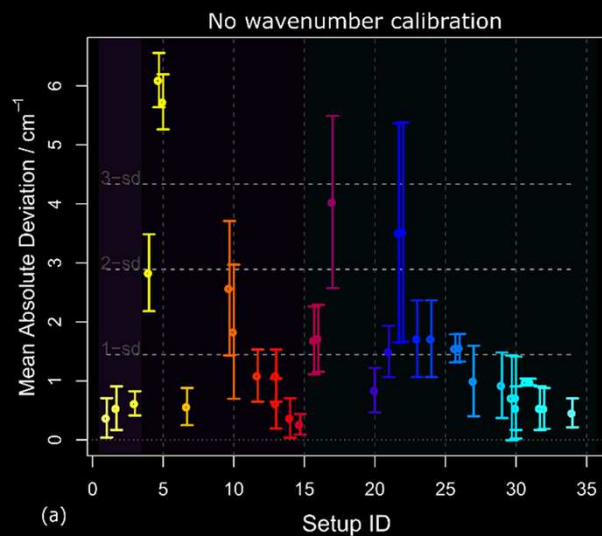
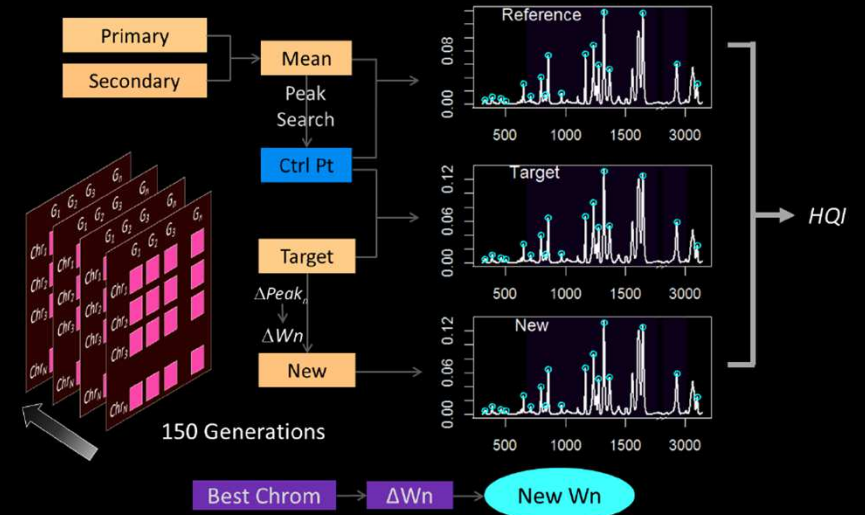


Reusable

Current State



Combination of Diverse Data – Data Standardization

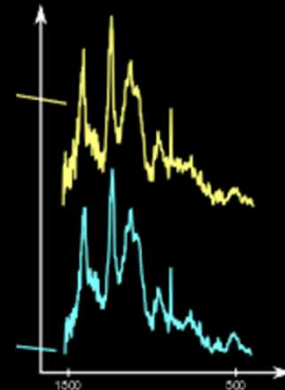
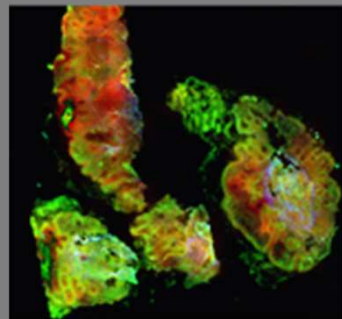
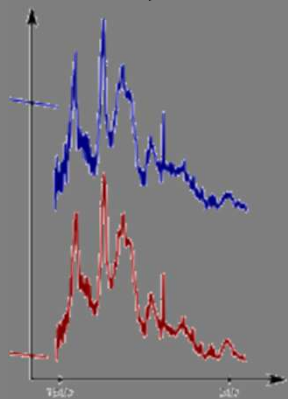


Combination of Diverse Data – Possible Solutions & Problems

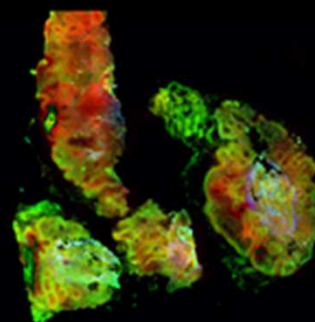
RDMoE system



Metadata



1D



2D



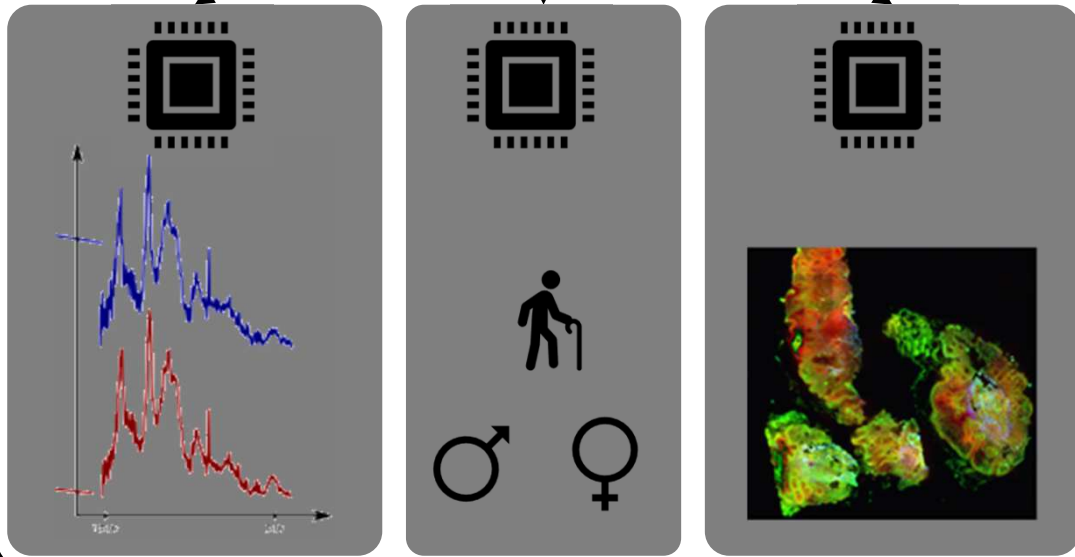
Differing Requirements

Combination of Diverse Data – Possible Solutions & Problems

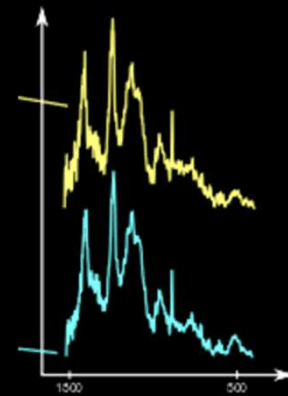
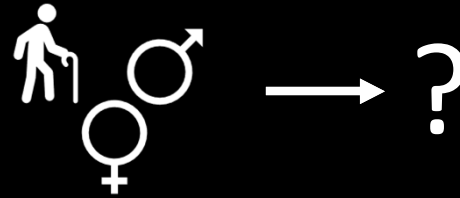
RDMoAE system



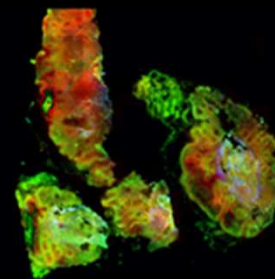
Metadata



What is a Scan?



400 –
3200 cm^{-1}



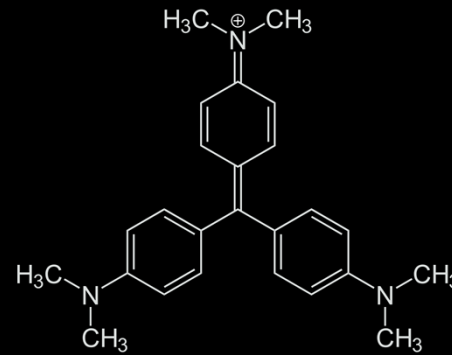
(-10,10) –
(25,40) μm



Differing
Metadata
Terminology

Combination of Diverse Data – Possible Solutions & Problems

! Differing Metadata Terminology

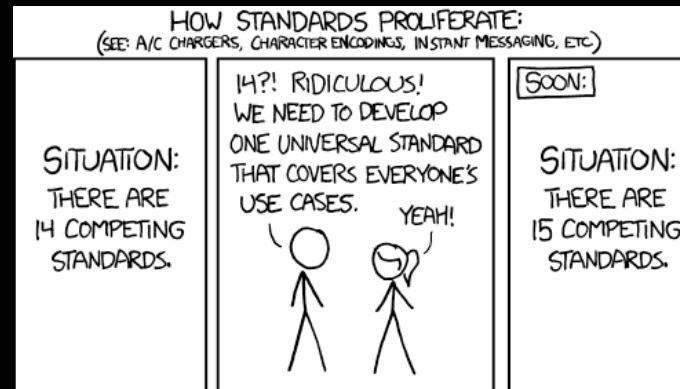
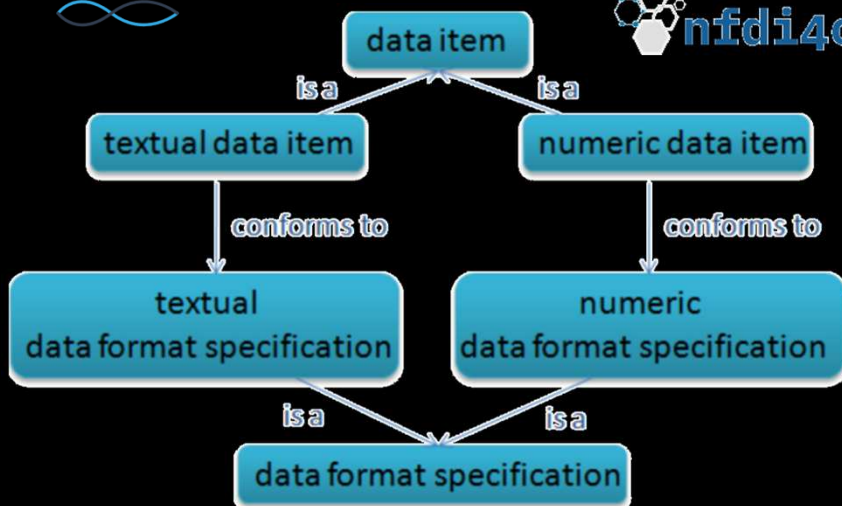


Crystal violet

{4-[4,4'-Bis(dimethylaminophenyl)benzhydrylidene]cyclohexa-2,5-dien-1-ylidene}dimethylammoniumchlorid

Ontology

FAIR




Differing Metadata Terminology !

Combination of Diverse Data – Possible Solutions & Problems

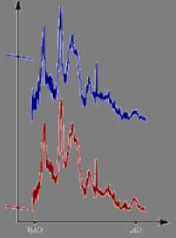
RDMoS system




Sample Metadata




Metadata



adroit



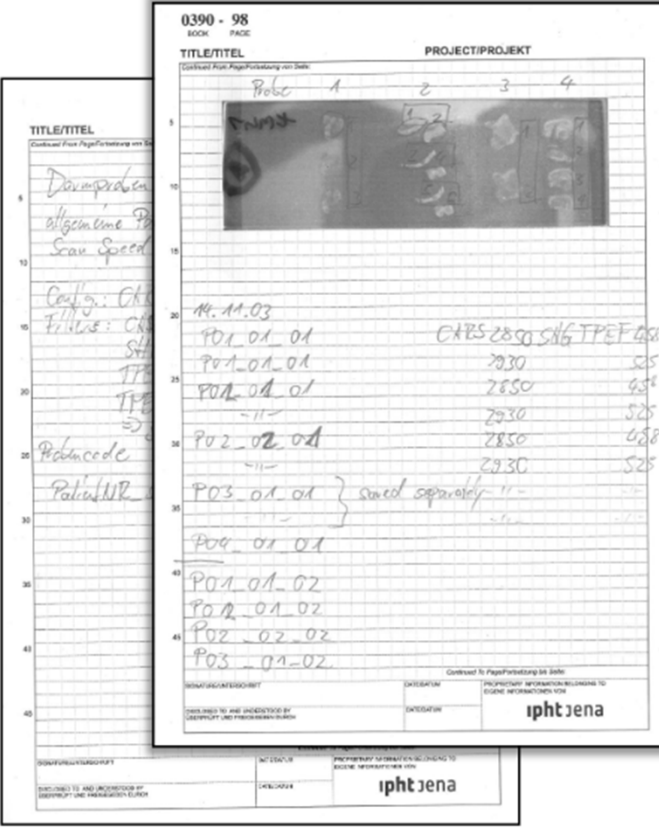
OMERO

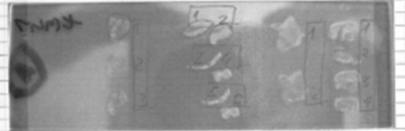


Metadata



Sample Metadata ?




BOOK	PAGE	PROJECT/PROJEKT		
0390	98			
TITLE/TITEL				
Continued from Page/fortsetzung von Seite				
	1	2	3	4
Pole				
				
Mr. M. 03				
CARB-2890-SHG-TPEF-450				
PO1_01_01 2830 525				
PO1_01_01 2850 654				
PO1_01_01 2930 525				
PO2_02_01 2850 658				
PO2_02_01 2930 525				
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PO4_01_01				
PO1_01_02				
PO2_01_02				
PO2_02_02				
PO3_01_02				



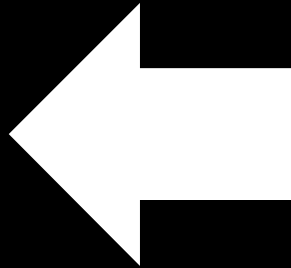
Sample Metadata
not easily accessible

Combination of Diverse Data – Possible Solutions & Problems

 **Sample metadata not easily accessible**



API



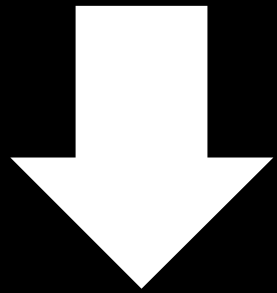
Measurement Data

Device: Which Device are you measuring on and in which configuration was it used?
Please fill out the table for each measurement you're taking

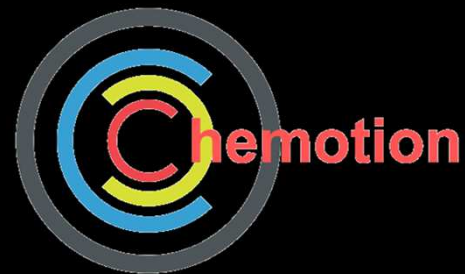
Sample Label	FileName	Running Number of Measurement	Acquisition Time	Number of Accumulations	Special Annotation	Use for Chemometrics
JH_EC11	JH_EC11_1.txt	1	10s	5	Spectra looks poor	n
JH_EC11	JH_EC11_2.txt	2	30s	5	Spectra looks good now	y
JH_EC11	JH_EC11_3.txt	3	30s	5		y
JH_EC12	JH_EC12_1.txt	1	30s	5		y
JH_EC12	JH_EC12_2.txt	2	30s	5		y
JH_EF11	JH_EF11_1.txt	1	30s	5		y
JH_EF11	JH_EF11_2.txt	2	30s	5		y
JH_Burk11	JH_Burk11_1.txt	1	30s	5		y
JH_Burk11	JH_Burk11_2.txt	2	30s	5		y

For Chemometrics - List of Samples with Batches

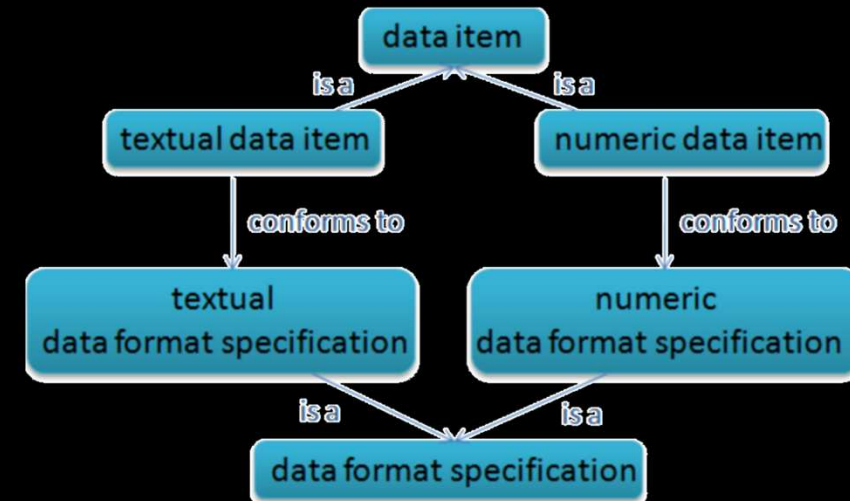
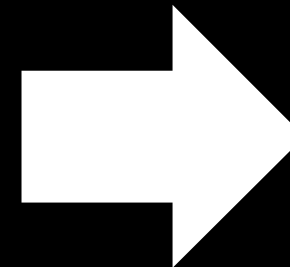
Sample	Genus	Species	Batch
JH_EC11	Escherichia	Coli	1
JH_EC12	Escherichia	Coli	2
JH_EF11	Escherichia	fergusonii	1
JH_Burk1	Burkholderia	Mallei	1



Sample metadata easily accessible



Different terminologies between groups



Combination of Diverse Data – Possible Solutions & Problems

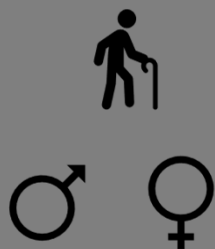
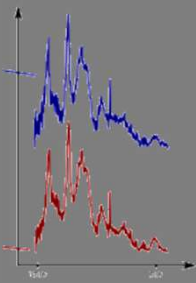
DIY RDM



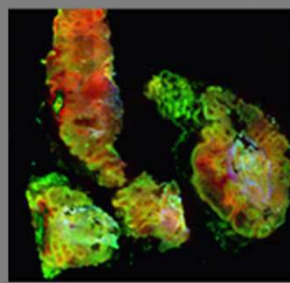
Metadata



Metadata



Metadata



Function
<code>GET.elabftw.byselector</code>
<code>GET.elabftw.bycaption</code>
<code>parseTable.elabftw</code>



Basically no infrastructure necessary



Can be implemented for existing data



Requires very good individual documentation to be FAIR

Summary

 **Findable**

 FAIRsharing.org
standards, databases, policies

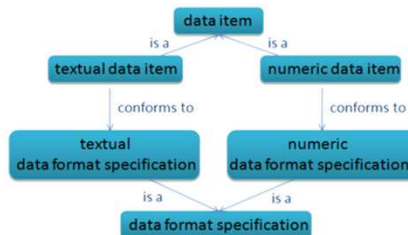
 nfdi4chem

 **Accessible**

 eLabFTW

 OME

 **Interoperable**



 **Reusable**



Q
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